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Non-equilibrium tunneling effects of interacting Hubbard–Anderson impurities

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Abstract. Non-equilibrium interaction effects of Hubbard-Anderson impurities have been experimentally studied by means of STM/STS methods and theoretically analyzed using self-consistent approach based on Keldysh formalism.

In this work, the interaction of the localized impurity states formed by a pair of identical impurity Si 3 nm apart at the (110) GaAs surface are studied by scanning tunneling microscopy and spectroscopy (STM/STS). In the experimentally observed spatial distribution of the local tunneling conductivity, one can recognize a two-fold switching on and off of each of atomic a and b states upon changing the tunneling bias. After switching on, the excess tunneling conductance occurs in the vicinity of each of these atoms in a bias range about 0.75 eV, which is much greater than the level width of localized state. At the same time, the transition from one state to other occurs upon changing bias in the range of 0.15 eV, which is comparable to the energy level width of the localized state.

Such effects have not been observed for individual impurity. We suggests self-consistent theoretical analysis of local tunneling conductivity behavior in the vicinity of two interacting Anderson impurities on semiconductor surface [1].

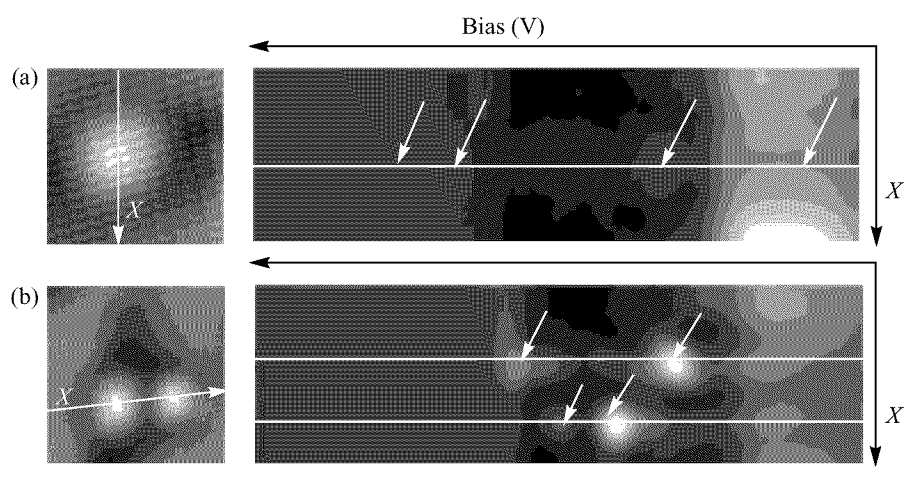

Fig. 1. STM images (right panel) and map view of normalized tunneling conductivity measured along direction depicted on STM topography images (left panel). Specific features on STS images are marked by arrows. (a) Isolated Si impurity, scan area 5.8 nm, bias range from +2.5 V to −2 V, (b) two interacting Si impuriies scan area 10 nm, bias range from +2.9 V to −2 V.

The influence of tunneling bias voltage on the impurity states energy values is taken into account. Non-equilibrium electron filling numbers on Hubbard–Anderson impurities are obtained from self-consistent system of kinetic equations based on Keldysh diagram technique. Coulomb interaction of localized electrons is treated self-consistently in mean-field approximation and is determined by these non-equilibrium filling numbers. It is shown that with increasing of tunneling bias two states with different energies for opposite spin electrons can appear on each impurity: the transition from "paramagnetic" regime to "magnetic" one can occur. The inverse transition from "magnetic" to "paramagnetic" state can also occur with further increasing of tunneling bias. We have also determined the conditions for enhancement of transition to magnetic state by increasing of interaction between two Anderson impurities. We revealed that impurity interaction results in redistribution of localized non-equilibrium charges and can lead to pinning of impurity levels near the Fermi level of each electrode and to mutual attraction of energy levels of different impurities in particular range of applied bias.

Non-equilibrium two impurity Anderson model is analyzed in mean-field approximation.

1. Mixed valence regime is considered $\varepsilon/\Gamma \geq 1$, $U \gg \varepsilon, \Gamma$.
ε, Γ are energy value and broadening of impurity state, U is on-site Coulomb interaction. Electron filling numbers n_σ and $n_{-\sigma}$ can differ from 0 and 1.

If $\Gamma \ll \varepsilon$ and the influence of tunneling interaction with the banks of the contact on impurity spectrum is neglected one obtain Coulomb blockade regime with n_σ and $n_{-\sigma}$ equal to 0 or 1 for $U \gg \varepsilon \gg \Gamma$. For Kondo regime $U \gg \varepsilon \gg \Gamma$ and the influence of tunneling interaction and electron correlation on quasi-particle spectrum in the banks of the contact and on impurity spectrum is taken into account. But in this case impurity level lies deep below E_F, n_σ and $n_{-\sigma}$ are also equal to 0 or 1.

2. Tunneling and relaxation rates γ_a, γ_b, γ_k are not infinite, so electron filling numbers n_σ and $n_{-\sigma}$ are non-equilibrium.

3. Energy values of impurity states are treated in self-consistent mean-field approximation $\varepsilon_\sigma^a(V, n_{-\sigma}^a(V)) = \varepsilon_a + \alpha V + U\langle n_{-\sigma}^a \rangle$.

4. Enchantment of tunneling conductivity with changing of tunneling bias voltage can be observed when $|\varepsilon_a^{\pm\sigma}(V) - E_F^t| < \Gamma$ or $|\varepsilon_a^{\pm\sigma}(V) - E_F^s| < \Gamma$.

Any increasing of LDOS at energy value $E_F - eV < \varepsilon < E_F$ when changing applied bias V leads to enhancement of tunneling conductivity at eV which can differ from ε.

Self consistent analysis of suggested model allows to distinguish different regimes of tunneling conductivity behaviour in the vicinity of impurity atoms with changes of tunneling bias.

(i) If $\gamma_k \ll \gamma_a, \gamma_b$ one of impurity atoms (atom a) can be in "magnetic" state in certain range of tunneling bias. With changing of applied voltage transition from "paramagnetic" regime to "magnetic" one and vise versa can occur. This behavior leads to switching "ON" and "OFF" twice of a atom on spatially resolved local tunneling conductivity spectra.

Besides energy levels are pinned in vicinity of Fermi level of one of electrodes (tip or sample) while bias voltage changes in the range of order of U.

In non-equilibrium case, when tunneling bias in not zero interaction between atoms a and b can enhance "magnetic" state and increase difference between energy values ε_σ and $\varepsilon_{-\sigma}$ of electrons with opposite spins localized on atom a.

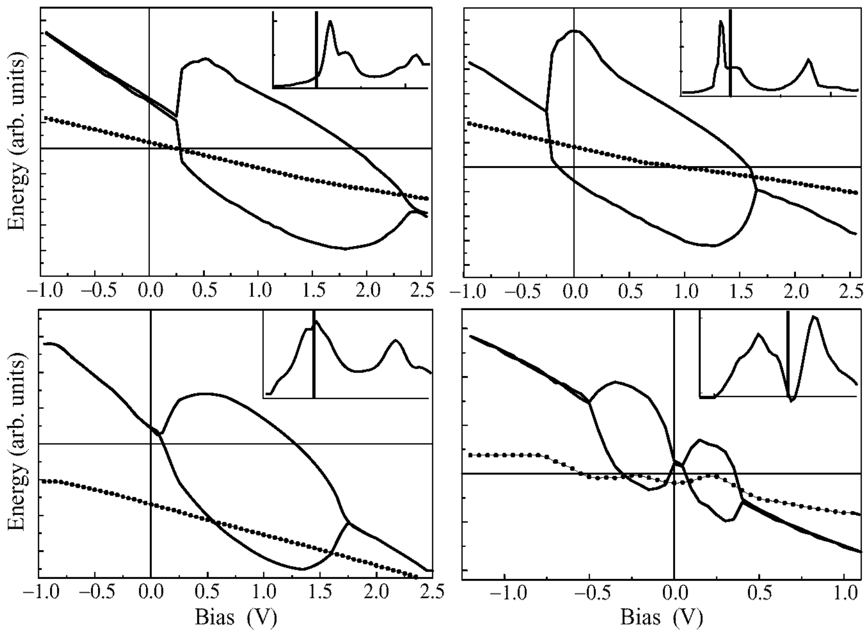

Fig. 2. Behavior of atoms a and b energy levels vs. tunneling bias for different parameters of tunneling junction. Two left graphs correspond to weak coupling to STM tip. Upper right graph corresponds to noninteracting impurity atoms, while lower one — to strong coupling to STM tip. Inserts show corresponding calculated normalized differential tunneling conductivity for the same bias range.

Detailed analysis of tunneling bias V range $|\varepsilon_a^{-\sigma}(V, n_a^\sigma) - E_F^s| < \Gamma$ leads to the following conclusions.

When there is no interaction between atoms (bias range $|\varepsilon_a^{-\sigma}(V, n_a^\sigma) - E_F^s| < \Gamma$) the state $\varepsilon_a^{-\sigma}(V, n_a^\sigma)$ is filling and $n_a^{-\sigma}(V)$, $\varepsilon_a^\sigma(V)$ are increasing, consequently $n_a^\sigma(V)$ and $\varepsilon_a^{-\sigma}(V)$ are decreasing. Levels $\varepsilon_a^{-\sigma}(V, n_a^\sigma)$ and $\varepsilon_a^\sigma(V, n_a^{-\sigma})$ become closer and sharp transition from "magnetic" to "paramagnetic" state occurs (Fig. 2(b)).

In presence of interaction filling of state $\varepsilon_a^{-\sigma}(V, n_a^\sigma)$ is suppressed due to charge redistribution between two interacting atom a and b. Correspondingly, increasing of $\varepsilon_a^\sigma(V, n_a^{-\sigma})$ and decreasing of $\varepsilon_a^{-\sigma}(V, n_a^\sigma)$ is also going slower than in non-interacting case. Thus the range of applied bias when atom a is in "magnetic" state become wider because of interatomic interaction (Fig. 2(a)). Let us stress the fact that this enhancement of "magnetic" regime is possible only in non-equilibrium case, i.e. for nonzero tunneling bias, and when energy levels $\varepsilon_{a(b)}^{\pm\sigma}(V, n_{a(b)}^{\mp\sigma})$ are close to the Fermi level of one of the electrodes.

In equilibrium case interaction with paramagnetic atom b will result in suppression of "magnetic" state on atom a (Fig. 2(a)).

Figure 2(c) depicts the dependence of tunneling conductivity on applied bias in vicinity of a atom. Two wide peaks on tunneling conductivity spectra correspond to switching "ON" of a atom at $\varepsilon_a^\sigma(V, n_a^{-\sigma}) = E_F^t$ and $\varepsilon_a^{-\sigma}(V, n_a^\sigma) = E_F^s$.

(ii) For $\gamma_k >> \gamma_a, \gamma_b$ (sufficiently strong coupling to STM tip) the situation when "magnetic" state on a atom appears twice is possible. In Fig. 2(d) the dependence of

$\varepsilon^{\pm\sigma}_{a(b)}(V, n^{\mp\sigma}_{a(b)})$ on applied bias is shown. In the range of applied bias $|\varepsilon^{\sigma}_{a}(V, n^{-\sigma}_{a}) - E^{s}_{F}| < \Gamma$ atom a is in the "magnetic" state. But with increasing of tunneling bias, filling numbers quickly decrease and "magnetic" regime is suppressed, and atom a can be found in "paramagnetic" state. However at opposite polarity of applied bias atom a can again be found in "magnetic" state when $|\varepsilon^{\sigma}_{a}(V, n^{-\sigma}_{a})$ is close to the Fermi level of the tip $|\varepsilon^{\sigma}_{a}(V, n^{-\sigma}_{a}) - E^{t}_{F}| < \Gamma$. Interaction between a and b atom can enhance this transition.

(iii) And finally, when coupling to the STM tip is comparable with coupling of impurity atom to the substrate $\gamma_k \geq \gamma_a, \gamma_b$ increasing of tunneling bias usually leads to suppression of "magnetic" state because filling numbers decrease due tunneling processes. Thus, we demonstrate the crucial rope of non-equilibrium effects in interacting bound tunneling nanostructures.

References

[1] P. I. Arseev, N. S. Maslova, S. I. Oreshkin, V. I. Panov and S. V. Savinov, *JETP Lett.* **72**, 121, 565, (2000).